

California – Denmark Conference
"Rational Design of Catalytic Materials"

14-15 January 2008

Lawrence Berkeley National Laboratory

The Experimental Basis for Rational Design of Heterogeneous Catalysts

Bjerne S. Clausen, Haldor Topsøe, Kgs. Lyngby, Denmark

Key words: catalysis, experimental techniques, in situ, operando, electron microscopy, EXAFS

Presentation Abstract

The establishment of relationships between the atomic structure and the reactivity of structurally complex heterogeneous catalysts is a prerequisite for a more rational design of catalytic materials. In order to get this information, *in situ* or *operando* investigations of catalysts under near realistic reaction conditions are needed, since the structure of the active catalyst is usually different from that found *ex situ* or *post mortem*. Most techniques have difficulties in coping with both the structural complexity of catalysts and with the fact that the studies should be carried out at conditions not too remote from those usually encountered in the catalytic reactor. During the last couple of decades, several *in situ* methods have been developed and successfully applied to gain insight into the active state of heterogeneous catalysts. Among the most successful methods introduced are X-ray absorption spectroscopy, X-ray diffraction, transmission electron microscopy, infrared and laser Raman spectroscopy. If appropriate *in situ*/reaction cells are applied it is possible not only to describe the detailed atomic structure *in situ* of nano-particle catalysts but also to record the catalytic activity simultaneously. This offers completely new opportunities for the establishment of relationships between the atomic structure and the reactivity of structurally complex heterogeneous catalysts. Examples of studies where the *in situ* conditions have been of decisive importance for the results obtained, will be described (e.g. 1-2).

References

1. P.L. Hansen, J.B. Wagner, S. Helveg, J. Rostrup-Nielsen, B.S. Clausen, and H. Topsøe, *Science*, 295 (2002) 2053.
2. S. Helveg, C. López-Cartes, J. Sehested, P.L. Hansen, B.S. Clausen, F. Abild-Pedersen, J.K. Nørskov, and J.R. Rostrup-Nielsen, *Nature* 427 (2004) 426.